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# TRANSPORT PROPERTIES OF THE "EXCITONIC INSULATOR"

## II. Thermal Conductivity<sup>\*</sup>

by

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### ABSTRACT

The thermal conductivity of the excitonic insulator<sup>1</sup> is calculated in the semimetallic limit. At low temperatures the main scattering mechanism is assumed to be due to impurities. Despite a recent claim of "superthermal conductivity" of the system which can be described as a condensate of electron-hole pairs we find that the thermal conductivity is "well behaved." It is shown that the thermal conductivity in the semimetallic limit of the underlying two band model is almost identical to the thermal conductivity of a superconductor containing magnetic impurities as scatterers. The analogy stems from the fact that the thermodynamic properties in both cases are similar as was discussed recently.

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## I. Introduction

In this paper we continue the analysis of transport properties of the "excitonic insulator" which has been discussed recently in the literature<sup>1,2</sup>. In the preceding paper<sup>3</sup>, hereafter referred to as II, we have calculated the electrical conductivity of the excitonic phase in the semimetallic region where the valence band and the conduction band of the underlying model overlap. The main scattering mechanism at low temperatures is assumed to be due to impurities. In I we have discussed the influence of the impurities on the thermodynamic description of the excitonic phase. It was shown that the situation could be described completely within the framework of the Abrikosov-Gorkov theory originally developed for superconductors containing magnetic impurities<sup>4</sup>.

In this paper we investigate the thermal conductivity of the excitonic phase which can be described as a condensate of bound pairs of electrons and holes. The main reason for this investigation is that Kozlov and Maksimov have recently claimed "superthermal conductivity" for such a system<sup>5</sup>. Such a novel situation certainly would be of major experimental interest. However, we shall show in the course of this work that the thermal conductivity of the excitonic phase is "well behaved," in fact it is similar to the thermal conductivity of a superconductor containing paramagnetic impurities as scatterers<sup>6</sup>. The contradictory claim of reference 5 is based on the Landau criterion for superfluidity; the derivation of the criterion for the excitonic phase contains a serious mathematical error<sup>7</sup>.

To start with we shall first discuss Kubo's formulas for the transport coefficients. Measuring energies relative to the chemical potential the electric current  $\underline{j}$  and the heat current  $\underline{u}$  are defined as follows<sup>8</sup>

$$\begin{aligned}\underline{j} &= -\frac{\sigma}{e}(\underline{\nabla}\mu - \frac{\mu}{T}\underline{\nabla}T) - \frac{L_1}{T}\underline{\nabla}T \\ \underline{u} &= -\frac{L_1}{e}(\underline{\nabla}\mu - \frac{\mu}{T}\underline{\nabla}T) - \frac{L}{T}\underline{\nabla}T\end{aligned}\quad (1)$$

where  $\mu$  is the chemical potential,  $T$  the temperature and  $e$  the electronic charge;  $\sigma$  is the d.c. conductivity. The thermal conductivity  $\kappa$  is obtained from (1) by

$$\underline{u} = -\kappa \underline{\nabla}T \quad ; \quad \underline{j} = 0 \quad (2)$$

which leads to

$$\kappa = \frac{1}{T} \left( L - \frac{L_1^2}{\sigma} \right) \quad (3)$$

The d.c. conductivity  $\sigma$  has been calculated in the preceding paper whereas the transport coefficients  $L$  and  $L_1$  are given by<sup>8</sup> (we anticipate spherical symmetry)

$$\begin{aligned}L &= \frac{1}{3} \int_0^\infty dt \int_0^\beta d\lambda \langle \underline{u}(0) \underline{u}(t+i\lambda) \rangle \\ L_1 &= \frac{1}{3} \int_0^\infty dt \int_0^\beta d\lambda \langle \underline{j}(0) \underline{j}(t+i\lambda) \rangle\end{aligned}\quad (4)$$

Here  $\underline{u}$  and  $\underline{j}$  are the Heisenberg operators for the energy and electric currents, respectively. The brackets indicate a thermal as well as an average over impurities as discussed in I and II.

The two band model we shall use has been discussed in detail in I and the preceding paper (II). The single particle energies in the two bands are assumed to be given near the Fermi surface by (see eq. (II.2))

$$\varepsilon_b(\underline{p}) = -\varepsilon_a(\underline{p}) = \frac{\underline{p}^2 - p_F^2}{2m} \quad , \quad (5)$$

where for mathematical convenience we assume equal band masses. We shall see later on that in the semimetallic limit (large  $p_0$ ) the thermoelectric coefficient  $L$ , is smaller by a factor  $k_B T / \frac{p_0^2}{2m}$  as compared to  $L$ . As we shall systematically neglect such terms, we confine our attention to the calculation of the coefficient  $L$ .

Another useful representation of  $L$  can be derived from the Kubo formula (4)<sup>9</sup>. Consider the causal correlation function

$$P(\tau_1 - \tau_2) = \frac{1}{\beta} \langle T \sum_m u(\tau_1) u(\tau_2) \rangle \quad (6)$$

where  $\tau_{1,2}$  are imaginary times with  $0 \leq \tau_{1,2} \leq \beta$ . Fourier transforming according to

$$P(\tau_1 - \tau_2) = \frac{1}{\beta} \sum_{\nu} P(i\nu) e^{-i\nu(\tau_1 - \tau_2)}, \quad \nu = 2n\pi\beta^{-1}, \quad (7)$$

we continue the discrete imaginary frequencies  $i\nu$  to the full complex energy plane. The coefficient is then given by

$$L = \frac{1}{2} \lim_{\omega \rightarrow 0} \frac{1}{i\omega} [P(\omega + i\delta) - P(\omega - i\delta)] = \lim_{\omega \rightarrow 0} \frac{1}{\omega} \text{Im} P(\omega + i\delta) \quad (8)$$

where  $\delta$  is a positive infinitesimal.

However, we have to be careful in using this formula for answering the question of "superthermal conductivity." This is because the mixing of "retarded" and "advanced" response in formula (8) neglects the possibility of an anomalous behavior of the real part of  $P(z = \omega + i\delta)$  in the limit  $\omega \rightarrow 0$ . Similar to the problem of infinite conductivity in superconductors, we expect that the possibility of an undamped heat current which could be accelerated by the temperature gradient would show up in the real part of the retarded correlation function  $P(\omega + i\delta)$  (thus leading to:  $\frac{\partial}{\partial t} u = \text{const.} \frac{\nabla T}{T}$ ). Instead of

formula (8) we shall consider the following expression

$$L = \lim_{\omega \rightarrow 0} \frac{P(\omega+i\delta) - C}{i\omega} \quad (9)$$

where the constant  $C$  will be determined later on by comparison with the corresponding expression for the normal state behavior. Formula (9) bears resemblance to the familiar expression for the electrical conductivity (see preceding paper).  $P(\omega+i\delta)$  would correspond to the paramagnetic contribution to the electric current (denoted by  $K^P(\omega+i\delta)$  in II) whereas the constant  $C$  would be equivalent to the diamagnetic contribution (denoted by  $-K^D$  in II)<sup>10</sup>.

In section II we derive a tractable form for  $P(i\nu)$  not dwelling on additive constants which are assumed to be absorbed in the constant  $C$ . In section III we make an ansatz for the constant  $C$  based on the required form in the normal state. We also shall be guided by the corresponding expression for the diamagnetic contribution in the problem of electrical conductivity. The resulting expression for the thermal conductivity will turn out to be "well behaved" as  $\omega \rightarrow 0$ . Thus there is no "superthermal conductivity." In section IV we calculate the final expression in analogy to calculations in the preceding paper. Section V contains explicit evaluations in several limits.

## II. Derivation of the heat current correlation function

The model has been discussed in detail in papers I and II (see section II of preceding paper). Denoting creation and annihilation operators for a- and b- electrons by  $\underline{a}_\rho^+, \underline{a}_\rho$  and  $\underline{b}_\rho^+, \underline{b}_\rho$  respectively we have introduced a Nambu notation

$$\underline{\psi}(\underline{p}) = \begin{pmatrix} \underline{b}_\rho \\ \underline{a}_\rho \end{pmatrix} ; \quad \underline{\psi}^+(\underline{p}) = \begin{pmatrix} \underline{b}_\rho^+ & \underline{a}_\rho^+ \end{pmatrix} . \quad (10)$$

The electric current operator has been written as (eq. II.19)

$$\underline{J}(\tau) = e \sum_{\underline{p}} \bar{\underline{\psi}}(\underline{p}, \tau) \hat{\underline{v}}(\underline{p}) \underline{\psi}(\underline{p}, \tau) \quad (11)$$

where the velocity matrix  $\hat{\underline{v}}(\underline{p})$  is explicitly

$$\hat{\underline{v}}(\underline{p}) = \begin{pmatrix} \underline{v}_b(\underline{p}) & 0 \\ 0 & \underline{v}_a(\underline{p}) \end{pmatrix} ; \quad \underline{v}_{a,b}(\underline{p}) = \frac{\partial}{\partial \underline{p}} \varepsilon_{a,b}(\underline{p}) . \quad (12)$$

Similarly the spatially uniform heat current operator can be defined by<sup>11</sup>

$$\underline{U}(\tau) = \frac{1}{2} \left( \frac{\partial}{\partial \tau'} - \frac{\partial}{\partial \tau} \right) \sum_{\underline{p}} \bar{\underline{\psi}}(\underline{p}, \tau') \hat{\underline{v}}(\underline{p}) \underline{\psi}(\underline{p}, \tau) \Big|_{\tau'=\tau+\gamma} \quad (13)$$

where  $\tau, \tau'$  are imaginary times and  $\gamma$  a positive infinitesimal indicating the ordering of operators. Expression (13) is the appropriate form when dealing with imaginary times in which case the Heisenberg field operators are given by equation (II.8) of the preceding paper. Introducing (13) into the correlation function (6) we obtain

$$P(\tau_1, \tau_2) = \frac{1}{12} \left( \frac{\partial}{\partial \tau_1'} - \frac{\partial}{\partial \tau_1} \right) \left( \frac{\partial}{\partial \tau_2'} - \frac{\partial}{\partial \tau_2} \right).$$

$$\cdot \sum_{\underline{p}, \underline{p}'} \left\langle T \bar{\psi}(\underline{p}, \tau_1') \hat{v}(\underline{p}) \psi(\underline{p}, \tau_1) \bar{\psi}(\underline{p}', \tau_2') \hat{v}(\underline{p}') \psi(\underline{p}', \tau_2) \right\rangle \Big|_{\substack{\tau_1' = \tau_1 + \delta \\ \tau_2' = \tau_2 + \delta}} \quad (14)$$

Actually the time derivatives in this expression should have been included in the brackets, as they do not commute with the time ordering operator  $T$ . By taking these derivatives outside we have neglected a term proportional to the  $\delta$ -function  $\delta(\tau_1 - \tau_2)$ . When Fourier transformed this correction term gives a constant which we assume to have been included in the constant  $C$  in equation (9).

The further calculation proceeds in a way similar to the calculation of the electrical current correlation function in the preceding paper. Introducing Greens functions (see I and II) and neglecting vertex corrections for a moment we get

$$\bar{P}(\tau_1, \tau_2) = -\frac{1}{12} \left( \frac{\partial}{\partial \tau_1'} - \frac{\partial}{\partial \tau_1} \right) \left( \frac{\partial}{\partial \tau_2'} - \frac{\partial}{\partial \tau_2} \right) \cdot \sum_{\underline{p}} \text{Trace} \hat{v}(\underline{p}) \underline{G}(\underline{p}, \tau_1 - \tau_1') \hat{v}(\underline{p}) \underline{G}(\underline{p}, \tau_2 - \tau_2') \Big|_{\substack{\tau_1' = \tau_1 + \delta \\ \tau_2' = \tau_2 + \delta}} \quad (15)$$

Fourier transforming we obtain

$$\bar{P}(iy) = -\frac{1}{12} \frac{\partial^2}{\partial \gamma^2} \frac{1}{\beta} \sum_{\underline{p}, \omega} \text{Trace} \hat{v}(\underline{p}) G(\underline{p}, i\omega_n) \hat{v}(\underline{p}) G(\underline{p}, i\omega_n - iy) e^{(2i\omega_n - iy)\gamma} \Big|_{\gamma=0} \quad (16)$$

where the time derivatives have been written as derivatives with respect to  $\gamma$ .

Comparing this expression with the electrical current correlation function

$K^P(iy)$  (II.21) we see that both are identical except for the prefactor, the  $\gamma$ -exponential and  $\gamma$ -derivatives and except that we have left out the vertex correction for the velocity matrix in (16). The vertex corrected expression  $P(iy)$  may be written down immediately from this comparison with (II.21):

$$P(iy) = -\frac{1}{12} \frac{\partial^2}{\partial \gamma^2} \frac{1}{\beta} \sum_{\underline{p}, \omega} \text{Trace} \hat{v}(\underline{p}) G(\underline{p}, i\omega_n) W(\underline{p}; i\omega_n, i\omega_n - iy) G(\underline{p}, i\omega_n - iy) e^{(2i\omega_n - iy)\gamma} \Big|_{\gamma=0} \quad (17)$$

where  $\underline{W}$  has been calculated in section III of the preceding paper. We remark that as usual the  $\omega$ -summation has to be performed first as the double summation converges only conditionally. Expression (17) is our final form of the heat current correlation function. The constant  $C$  which according to equation (9) has to be subtracted from (17) will be considered in the following section.

### III. Determination of the subtraction constant

We shall determine the subtraction constant  $C$  in formula (9) by analogy from the corresponding constant in the electrical conductivity problem, i.e. the diamagnetic contribution. The latter is given from equation (II.18) of the preceding paper

$$-K^D = \frac{e^2}{3} \sum_{\underline{p}} \left[ (\nabla_{\underline{p}}^2 \epsilon_b(\underline{p})) n_b(\underline{p}) + (\nabla_{\underline{p}}^2 \epsilon_r(\underline{p})) n_a(\underline{p}) \right], \quad (18)$$

where the  $\epsilon_{a,b}$  are the general band energies,  $n_{a,b}(\underline{p})$  the occupation numbers in

momentum space. We rewrite the occupation numbers in terms of the spectral functions<sup>12</sup>

$$n_{a,b}(\underline{p}) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f(\omega) S_{a,b}(\underline{p}, \omega) \quad (19)$$

where  $f(\omega)$  is the Fermi distribution function, and the spectral functions are expressed through the one-particle Greens functions

$$S_{a,b}(\underline{p}, \omega) = i \left[ G_{a,b}(\underline{p}, \omega + i\delta) - G_{a,b}(\underline{p}, \omega - i\delta) \right] \quad (20)$$

Thus we can write for (18)

$$-K^D = \frac{1}{3} \sum_{\underline{p}} (\nabla_{\underline{p}}^2 \varepsilon_b(\underline{p})) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^2 f(\omega) S_b(\underline{p}, \omega) + (b \rightarrow a) \quad (21)$$

The product  $f(\omega) S_b(\underline{p}, \omega)$  can be interpreted as the density of particles with momentum  $\underline{p}$  and energy  $\omega$ .

It is intuitively clear that in the thermal conductivity problem we should replace the charge  $e$  in expression (21) by the energy  $\omega$ . Therefore we make the following ansatz for the constant  $C$ :

$$\begin{aligned} C &= \frac{1}{3} \sum_{\underline{p}} (\nabla_{\underline{p}}^2 \varepsilon_b(\underline{p})) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega^2 f(\omega) S_b(\underline{p}, \omega) + (b \rightarrow a) \\ &= \frac{1}{3} \frac{\partial^2}{\partial \gamma^2} \sum_{\underline{p}} (\nabla_{\underline{p}}^2 \varepsilon_b(\underline{p})) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{e^{\gamma \omega}}{e^{\beta \omega} + 1} i \left[ G_b(\underline{p}, \omega + i\delta) - G_b(\underline{p}, \omega - i\delta) \right] \Big|_{\gamma=0} + (b \rightarrow a) \end{aligned} \quad (22)$$

where in the second line we have explicitly introduced the functions  $f$  and  $S$ . The  $\omega^2$ -factor is generated by the  $\gamma$ -derivatives, and  $\gamma$  is a small positive number which has to be set equal to zero finally as indicated in (22).

The  $\omega$ -integral can be transformed into a summation over imaginary frequencies  $i\omega_n$ . This is done by closing the contour of the integral for the first integrand in (22) by a large semicircle in the upper half plane and for

the second integrand in the lower half plane. Summing over the residues at the poles of the Fermi function at  $z = i\omega_n = i(2n+1)\pi\beta^{-1}$  we get at once:

$$C = \frac{1}{3} \frac{\partial^2}{\partial \delta^2} \frac{1}{\beta} \sum_{\underline{p}\omega} (\nabla_{\underline{p}}^2 \epsilon_b(\underline{p})) G_b(\underline{p}, i\omega_n) e^{i\omega_n \delta} \Big|_{\delta=0} + (b \rightarrow a), \quad (23)$$

where the  $\omega$ -summation has to be performed first as usually. In order to make contact with the correlation function expression (17), the right hand side in (23) is further transformed by a partial  $\underline{p}$ -integration over the Brillouin zone. In analogy to the calculation in the preceding paper (eq. II.22) we get

$$C = -\frac{1}{3} \frac{\partial^2}{\partial \delta^2} \frac{1}{\beta} \sum_{\underline{p}\omega} v_b(\underline{p}) \frac{\partial}{\partial \underline{p}} G_b(\underline{p}, i\omega_n) e^{i\omega_n \delta} \Big|_{\delta=0} + (b \rightarrow a) \quad (24)$$

where  $v_{b,a}(\underline{p})$  are the group velocities  $\frac{\partial}{\partial \underline{p}} \epsilon_{b,a}(\underline{p})$  (12). Using the Greens functions of the preceding paper (II.9), we have after taking the derivatives and combining all terms in analogy with expression (II.23):

$$C = -\frac{1}{12} \frac{\partial^2}{\partial \delta^2} \frac{1}{\beta} \sum_{\underline{p}\omega} \text{Trace} \hat{v}(\underline{p}) G(\underline{p}, i\omega_n) \hat{v}(\underline{p}) G(\underline{p}, i\omega_n) e^{2i\omega_n \delta} \Big|_{\delta=0}. \quad (25)$$

For better comparison with  $P(i\nu)$  (17) we also have substituted  $\delta \rightarrow 2\delta$ .

Comparing this expression with expression (17) for the correlation function  $P(i\nu)$  we see that

$$C \equiv P(i\nu=0), \quad (26)$$

because the vertex corrected velocity matrix  $\underline{W}$  in (17) reduces to the free vertex function  $\hat{v}$  at  $\nu=0$  (see equations (II.25,26,30) of the preceding paper). As the statement (26) is independent of the fact whether the system is in the normal state or the excitonic state, we can conclude quite generally that the thermal conductivity is "well behaved." This is because (26) guarantees that the real part of the numerator in (9) vanishes in the limit  $\omega \rightarrow 0$ . This

conclusion will be confirmed by the calculations in the next two sections.

#### IV. Evaluation of the thermal conductivity

Combining the two expressions (17) and (25) we can follow very closely the calculations of the corresponding expressions (II.21,23) in the preceding paper. We first perform the momentum integral evaluating the total expression at the Fermi surface. In analogy to the result (II.33) of the preceding paper we get

$$\rho(i\nu) \equiv P(i\nu) - C = -\frac{\rho}{2m} \frac{\partial^2}{\partial \delta^2} \frac{\pi}{\beta} \sum_{\omega} F(i\omega_n, i\omega_n - i\nu) e^{(2i\omega_n - i\nu)\delta} \Big|_{\delta=0} \quad (27)$$

where  $\rho$  is the density of electrons or holes, respectively, and the function  $F$  has been defined in equation (II.34). The further calculation differs slightly from the corresponding calculation in section IV of the preceding paper because of the presence of the  $\delta$ -exponential in (27). We write the frequency summation as a contour integral in the complex plane:

$$\frac{\pi}{\beta} \sum_{\omega} F(i\omega_n, i\omega_n - i\nu) e^{(2i\omega_n - i\nu)\delta} = -\frac{1}{2i} \int_{C_0} dz \frac{e^{(2z - i\nu)\delta}}{e^{\beta z} + 1} F(z, z - i\nu), \quad (28)$$

the path  $C_0$  being defined in equation (II.35) of the preceding paper. Because of the  $\delta$ -exponential we have to choose the Fermi function in (28) instead of the tanh-function in (II.35) in order to insure the vanishing of the integrand for large  $z$ . The integral (28) is further transformed into an integral over the discontinuities of the function  $F(z, z - i\nu)$  across its cuts. These cuts are defined in equation (II.37). The contribution from the first cut  $C_1$  is given by

$$J_1 = -\frac{1}{2i} \int_{\omega_c}^{\infty} dx \frac{e^{(2x - i\nu)\delta}}{e^{\beta x} + 1} [F(x + i\delta, x - i\nu) - F(x - i\delta, x - i\nu)] \quad (29)$$

where  $\omega_0$  is the gap in the excitation spectrum of the system (II.10). Similarly the contribution from the cut  $C_4$  gives

$$\begin{aligned} J_4 &= -\frac{1}{2i} \int_{iy-\infty}^{iy-\omega_0} dz \frac{e^{(2z-iy)\gamma}}{e^{\beta z} + 1} [F(z, z-iy+i\delta) - F(z, z-iy-i\delta)] \\ &= \frac{1}{2i} \int_{\omega_0}^{\infty} dx \frac{e^{-(2x-iy)\gamma}}{e^{-\beta x} + 1} [F(x+i\delta, x-iy) - F(x-i\delta, x-iy)] \end{aligned} \quad \begin{matrix} z \rightarrow iy-x \\ (30) \end{matrix}$$

where we have used (II.38). The contributions from the two cuts  $C_2$  and  $C_3$  can be transformed to integrals over the cut  $C_1$  in the same way. Combining all 4 terms and rearranging we obtain for the right hand side of (27)

$$\begin{aligned} p(iy) &= -\frac{\rho}{4mi} \frac{\partial^2}{\partial \gamma^2} \int_{\omega_0}^{\infty} dx \left\{ [F(x+i\delta, x-iy) - F(x-i\delta, x-iy)] \left[ \tanh \frac{\beta x}{2} \cosh(2x-iy)\gamma - \sinh(2x-iy)\gamma \right] \right. \\ &\quad \left. + [F(x+i\delta, x+iy) - F(x-i\delta, x+iy)] \left[ \tanh \frac{\beta x}{2} \cosh(2x+iy)\gamma - \sinh(2x+iy)\gamma \right] \right\} \Big|_{\gamma=0}. \end{aligned} \quad (31)$$

According to formula (9) we have to take the analytical continuation of this expression from  $z=iy$  to  $z=\omega+i\delta$  and then pass to the limit  $\omega \rightarrow 0$ . This process leads to the following expression for the transport coefficient  $L$ :

$$\begin{aligned} L &= \frac{\rho}{4m} \frac{\partial^2}{\partial \gamma^2} \lim_{\omega \rightarrow 0} \frac{1}{\omega} \int_{\omega_0}^{\infty} dx \left\{ F(x+i\delta, x-\omega-i\delta) \left[ \tanh \frac{\beta x}{2} \cosh(2x-\omega)\gamma - \sinh(2x-\omega)\gamma \right] \right. \\ &\quad \left. - F(x-i\delta, x+\omega+i\delta) \left[ \tanh \frac{\beta x}{2} \cosh(2x+\omega)\gamma - \sinh(2x+\omega)\gamma \right] \right\} \Big|_{\gamma=0} \end{aligned} \quad (32)$$

where we have left out the contributions from  $F(x-i\delta, x-\omega-i\delta)$  and  $F(x+i\delta, x+\omega+i\delta)$  which according to (II.42) vanish in the limit  $\omega \rightarrow 0$ . Furthermore we can transform  $x \rightarrow x+\omega$  in the first part of the integral and split the integration into two terms. The first of these terms is the integral from  $\omega_0-\omega$  to  $\omega_0$  and gives for small  $\omega$

$$\frac{1}{\omega} \int_{\omega_0-\omega}^{\omega_0} dx F(x+\omega+i\delta, x-i\delta) \left[ \tanh \frac{\beta(x+\omega)}{2} \cosh(2x+\omega)\gamma - \sinh(2x+\omega)\gamma \right]$$

$$\sim F(\omega_0+i\delta, \omega_0-i\delta) \left[ \tanh \frac{\beta\omega_0}{2} \cosh(2\omega_0\gamma) - \sinh(2\omega_0\gamma) \right] \equiv 0, \quad (33)$$

as discussed in equations (II.44,45) of the preceding paper. The second integral ( $\omega_0 \leq x < \infty$ ) can be combined with the second part in (32) leading to

$$L = \frac{p}{m} \frac{\partial^2}{\partial \gamma^2} \int_{\omega_0}^{\infty} dx \frac{\beta}{2} \operatorname{sech}^2 \frac{\beta x}{2} F(x+i\delta, x-i\delta) \cosh(x\gamma) \Big|_{\gamma=0} \quad (34)$$

where we have replaced  $2\gamma \rightarrow \gamma$ .

Comparing this expression with equations (II.46,47) of the preceding paper we see that the d.c. conductivity apart from the factor  $e^2$  may be obtained from (34) by leaving out the  $\gamma$ -derivatives. This is explained by the fact that the heat current (13) differs from the electric current (11) by the time derivatives which eventually are represented by the  $\gamma$ -derivatives in the correlation function expression (17). In the same way it is clear that the thermoelectric coefficient  $L_1$  (4) is given by (34) with one  $\gamma$ -derivative only, as there is only one heat current involved in the correlation function (4) for  $L_1$ <sup>13</sup>.

Therefore  $L_1$  obviously vanishes. The reason for this is that we have evaluated the momentum integral at the Fermi surface in passing from expression (17) to expression (27). Correction terms would be smaller by a factor  $K_B T / \frac{p_F^2}{2m}$  which we have neglected systematically. Thus the thermoelectric coefficient  $L_1$  is zero to a sufficient accuracy.

The thermal conductivity  $\kappa$  is therefore given from (3) and (34)

$$\kappa = \frac{\rho}{m} \frac{\beta}{T} \int_{u_0}^{\infty} dx x^2 \operatorname{sech}^2 \frac{\beta x}{2} \frac{h(x)}{2[\Delta J_m \sqrt{u^2 - 1} - \Gamma] + 2\Gamma'(1-h) + \Gamma_{tr}} \quad (35)$$

where we have introduced the function  $\frac{1}{2} F(x+i\delta, x-i\delta)$  from equation (II.48) of the preceding paper; the different terms and symbols are also explained in section V and the Appendix of the preceding paper. Explicit calculations in several limits are considered in the final section.

#### V. Discussion and explicit calculations

We may compare our final expression (35) with the corresponding formula for the thermal conductivity of a superconductor containing magnetic impurities as derived in reference 6 (equation (3.1)). The two expressions are identical if we replace the total density of particles  $\rho$  in the formula of reference 6 by

$2\rho$  in our case which is due to the two types of carriers. The similarity is not surprising as we have seen in reference 2 (paper I) that the excitonic phase in the presence of impurities has the same thermodynamic properties as a superconductor with magnetic impurities. Therefore one expects that the reaction to a temperature gradient is similar in both systems because the different charges of the bound pairs are not significant in this case.

The fact that the expression (35) is well behaved over the whole temperature range clearly disproves the claim of reference 5 that the excitonic phase should have "superthermal" properties. It remains to discuss the behavior of the thermal conductivity in several limits which are accessible to explicit calculations.

In the normal state ( $\Delta=0$ ) we obtain from (35) using (II.51) of the preceding paper

$$\kappa_n = \frac{2\pi^2 \rho \tau_{tr}}{3m} K_B^2 T \quad (36)$$

where  $\tau_{tr.} = \Gamma_{tr.}^{-1}$  is the transport collision time (II.50). Upon comparison with the "normal" conductivity (II.52) we have the Wiedemann-Franz law

$$\frac{\kappa_n}{\sigma_n} = \frac{\pi^2}{3} \frac{K_B^2 T}{e^2} . \quad (37)$$

Using (36) we write

$$\frac{\kappa}{\kappa_n} = \frac{3\beta^3 \Gamma_{tr.}}{2\pi^2} \int_{\omega_0}^{\infty} dx x^2 \operatorname{sech}^2 \frac{\beta x}{2} \frac{h(x)}{2[\Delta J_m \sqrt{\omega^2 - 1} - \Gamma] + 2\Gamma'(1-h) + \Gamma_{tr.}} . \quad (38)$$

In order to evaluate this expression asymptotically near  $T = 0$  we have to distinguish between the two cases whether the excitation spectrum of the system has a gap ( $\omega_0 \neq 0$ ) or not. In the first case, i.e. for low impurity concentration ( $\alpha = \frac{\Gamma}{\Delta} < 1$ , see the preceding paper), we obtain, using the expressions (II.54) and (II.55) of the preceding paper, respectively

$$\frac{\kappa}{\kappa_n} = \frac{4}{\pi^2} \frac{1 - \alpha^{2/3}}{\frac{2\Gamma}{\Gamma_{tr.}} - \alpha^{2/3}} \beta \omega_0 e^{-\beta \omega_0} , T \geq 0 , \alpha = \frac{\Gamma}{\Delta} < 1 . \quad (39)$$

Thus the thermal conductivity goes to zero exponentially as long as there is a gap in the excitation spectrum.

In the gapless region ( $\alpha > 1$ ) we get at  $T = 0$  using (II.58) of the preceding paper and starting the integration in (38) at  $\omega_0 = 0$

$$\frac{\kappa}{\kappa_n} = \frac{1 - \alpha^{-2}}{1 + \frac{2\Gamma'}{\Gamma_{tr.}} \alpha^{-2}} < 1 , \quad \alpha = \frac{\Gamma}{\Delta} > 1 . \quad (40)$$

Comparing with (II.59) we see that in the gapless region the ratio  $\kappa/\kappa_n$  is identical to the ratio  $\sigma/\sigma_n$  for the d.c. conductivity. Therefore the Wiedemann-Franz law holds, too.

Finally, we consider the transition temperature region where the system is always gapless ( $\alpha = \frac{r}{\Delta} > 1$  as  $\Delta \rightarrow 0$ ). Expanding (38) in powers of  $\Delta^2$  we conclude in analogy to equations (II.62,65) of the preceding paper that

$$\frac{x}{x_n} = 1 - \text{const} \cdot (1-t), \quad t = \frac{T}{T_c} \lesssim 1. \quad (41)$$

Numerical solutions for the superconductor case in the whole temperature range are reported in reference 6.

# REFERENCES

1. References to the theoretical work can be found in D. Jerome, T. M. Rice, and W. Kohn, Phys. Rev. 158, 462 (1967), and in reference 2.
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6. V. Ambegaokar and A. Griffin, Phys. Rev. 137, 1151 (1965).
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8. See for example: J. S. Langer, Phys. Rev. 128, 110 (1962).
9. See for example: V. Ambegaokar, in "Brandeis Lectures," 1962. (W. A. Benjamin, INC, New York, 1963) Vol. 2.
10. One might interpret the contribution  $P(\omega+i\delta)$  as being due to a change of the density matrix in the presence of a temperature gradient. The second contribution C could be regarded as being due to the fact that the heat current operator is different from the case where there is no "external field."

11. For the definition of the heat current see for example references 6 and 8.
12. L. P. Kadanoff and G. Baym "Quantum Statistical Mechanics." (W. A. Benjamin, INC, New York, 1962), Chapter 1 and 2.
13. For a similar discussion see reference 6.

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13. ABSTRACT The thermal conductivity of the excitonic insulator <sup>1</sup> is calculated in the semimetallic limit. At low temperatures the main scattering mechanism is assumed to be due to impurities. Despite a recent claim of "superthermal conductivity" of the system which can be described as a condensate of electron-hole pairs we find that the thermal conductivity is "well behaved." It is shown that the thermal conductivity in the semimetallic limit of the underlying two band model is almost identical to the thermal conductivity of a superconductor containing magnetic impurities as scatterers. The analogy stems from the fact that the thermodynamic properties in both cases are similar as was discussed recently.			

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